Benzenesulfonic acid, 3-hydrazino-138-30-7 | DTXSID8059681

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 271 °C

Global applicability domain: Outside

Local applicability domain index: 1.76e-01

Confidence level: 7.21e-01

Nearest Neighbors from the Training Set

Image not found

N-(4-Bromophenyl)urea

Measured: 260 Predicted: 256 Image not found

1-Phenylurea

Measured: 238 Predicted: 247 Image not found

Diphenylurea
Measured: 262
Predicted: 269

Image not found

Chloramben
Measured: 312
Predicted: 301